International Letters of Chemistry, Physics and Astronomy *Online: 2015-01-14*
ISSN: 2299-3843, Vol. 44, pp 130-140
doi:10.18052/www.scipress.com/ILCPA.44.130

Acoustical Studies of some Chalcones in DMF and DMSO Solutions

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ABSTRACT

This work reports densities, speeds of sound, and isentropic compressibility of the solutions of some synthesized chalcones in N,N-dimethylformamide and dimethyl sulphoxide solutions of various concentrations at 308.15 K with a view to understand molecular interactions in these solutions.

Keywords: Chalcones; sound velocity; isentropic compressibility

1. INTRODUCTION

Literature survey shows that because of its non destructive nature, ultrasonic waves have been used in various industries for various processes like dyeing[1], cleaning[2], design[3], bleaching[4], food processing[5], organic synthesis[6,7] etc. Further, it is also used in medical fields[8-10].

The ultrasonic measurements have also been used to study molecular interactions in various pure liquids[11], liquid mixtures[12,13] and solutions of organic and inorganic compounds[14-16], polymers[17], amino acids[18], drugs[19] etc. The thermodynamic parameters calculated through ultrasonic velocity measurements can give idea about intermolecular attraction between molecules (solute-solute or solute-solvent)[28].

In our laboratory, the ultrasonic and physicochemical studies of some organic compounds like Schiff bases[20], triazoles[21], dihydropyrimidines[22] etc. have been studied in different solvents. In continuation of our previous work, in the present paper, ultrasonic studies of some chalcones base have been studied in N, N dimethylformamide and dimethylsulphoxide solutions of various concentrations at 303.15 K with a view to understand molecular interactions in these solutions.

2. EXPERIMENTAL

The solvents N, N-dimethylformamide and dimethylsulphoxide were of analytical grade and were distilled by the reported procedure[23]. The purities of these solvents values were checked by a gas-liquid chromatography and were found to be 99.5% and 99.6% for N, N dimethylformamide and dimethyl sulphoxide respectively. The solvents were degassed and dried over molecular sieves (Union Carbide, type 0.4 nm).

The chalcones (ANC-1 to ANC-9) were synthesized in our laboratory and were recrystalized before use. The physical constants of all the synthesized chalcones are given in Table 1. The general structure of chalcone is given in Figure 1.

The densities, viscosities and ultrasonic velocities of pure solvents and solutions of chalcones of different concentrations were measured at 303.15 K by using pyknometer, an Ubbelohde suspended level viscometer and single frequency ultrasonic interferometer (Mittal Enterprises, Model No F81) operating at 2 MHz, with the uncertainties of 0.0001 g/cm^3, $\pm$ 0.06 % and 0.01% respectively. The temperature was maintained by an electronically controlled thermostatic water bath (NOVA NV-8550 E). The uncertainty of temperature was $\pm 0.1^{o}$ C.

All the solutions were prepared by using a Mettler Toledo AB204-S balance with a precision of (1×10^{-4}) g.

3. RESULTS AND DISCUSSION

Table 2 shows the experimental data of density (ρ), viscosity (η) and sound velocity (U) of pure solvents and solutions of chalcones in DMF and DMSO solutions at 303.15 K. From these experimental data, various acoustical parameters like specific acoustical impedance (Z), isentropic compressibility (κ_S), inter molecular free length (L_f), Rao's molar sound function (R_m), Vander Waals constant (b), relaxation strength (r), internal pressure (π), apparent molar compressibility (ϕ_k) etc., were evaluated using the equations reported earlier[20].

Some of the calculated acoustical parameters are given in Tables 3 and 4 for all the compounds in DMF and DMSO solutions respectively. Figure 2 shows the variation of ultrasound velocity *(U)* with concentration in DMF and DMSO respectively. It is observed that in both the solvents, ultrasonic velocity *(U)* increases non linearly with concentration for all the compounds. Whereas Figure 3 shows that intermolecular free length *(L_f)* decreases with concentration. Thus, ultrasonic velocity is reverse of intermolecular free length *(L_f)*. The decrease of intermolecular free length means the distance between solute (compound) and solvent molecules decreases i.e., strong interaction between solvents and compound molecules exists in these solvents which causes ultrasonic velocity to increase.

This is further supported by isentropic compressibility *(κ_S)* and relaxation strength *(r)*. The isentropic compressibility *(κ_S)* of the solutions in both the solvents is also found to decrease with increase of concentration, as shown in Figure 4. Due to solute-solvent interactions in the system, compressibility of the solution decreases with the increase in concentration. This is further confirmed by decrease of relaxation strength *(r)* and increase in specific impedance *(Z)* values (as reported in Tables 3 and 4). The Rao's molar sound function (R_m) and Vander Waal's constant *(b)* are also observed to increase linearly (correlation coefficient 0.9985-0.9998) with concentration for all the compounds in both the solvents. The linear increase of these parameters shows absence of complex formation in these systems.

The internal pressure is the result of forces of attraction and repulsion between molecules in a solution. As Tables 3 and 4 shows that internal pressure (π) decreases in both the solvents. This indicates that solute-solute interactions also exist in these solutions.

The predominance of solute-solvent interactions is further confirmed by evaluating some other parameters. The isentropic compressibility of all the solutions was also fitted to the following Bachem's relation[24]:

$$\kappa_s = \kappa_s^0 + AC + BC^{3/2}$$

From the plot of $\left(\kappa_s - \kappa_s^0\right)/C$ verses $\sqrt{C}$, values of A and B constants were evaluated from the intercept and slope respectively. κ_s^0 is the isentropic compressibility of pure solvent. Further, the apparent molar compressibility (ϕ_k) of the solutions is fitted to Gucker's relation25:

$$\phi_k = \phi^o{}_k + S_k \sqrt{C}$$

From the plot of ϕ_k verses $\sqrt{C}$, $\phi^o{}_k$ and S_k values are evaluated from the intercept and slope. S_k is known as interaction parameter.

It is evident from Table 5 that in both DMF and DMSO solutions, A and $\phi^o{}_k$, values are negative whereas B and S_k values are positive. The negative A and $\phi^o{}_k$ confirms interaction between solvent and compound molecules. Further, the positive values of B and S_k confirms the predominance of solute-solvent interactions in studied systems.

Thus, it is concluded that for the synthesized chalcones, although both solute-solute and solute-solvent interactions exist in these solutions, solute-solvent interactions dominate in both DMF and DMSO solutions.

Table 1. Physical constants of synthesized Chalcones.

Code	*R*	*M.F.*	*M.W.*	*Yield (%)*	*R_f value**
ANC-1	4-CH_3,C_6H_4-	$C_{24}H_{18}O$	322.40	62	0.46
ANC -2	4-OH-C_6H_4-	$C_{23}H_{16}O_2$	324.37	45	0.56
ANC -3	4-Br-C_6H_4-	$C_{23}H_{15}BrO$	387.27	69	0.49
ANC -4	4-F-C_6H_4-	$C_{23}H_{15}FO$	326.36	74	0.52
ANC -5	4-Cl-C_6H_4-	$C_{23}H_{15}ClO$	342.82	71	0.56
ANC-6	4-NO_2-C_6H_4-	$C_{23}H_{15}NO_3$	353.37	79	0.51
ANC -7	4-NH_2-C_6H_4-	$C_{23}H_{17}NO$	323.39	65	0.56
ANC -8	4-OCH_3-C_6H_4-	$C_{24}H_{18}O_2$	338.40	61	0.47
ANC -9	$C_9H_5O_2$-	$C_{26}H_{16}O_3$	376.40	59	0.58

*Hexane: Ethyl acetate-6.5:3.5

Table 2. The density (ρ), ultrasonic velocity (U) and viscosity (η) of Chalcones in DMF and DMSO.

Conc. M	*Density ρ g.cm^{-3}*	*Velocity U. 10^{-5} cm.s-1*	*Viscosity η.10^3 poise*	*Density ρ g.cm^{-3}*	*Velocity U. 10^{-5} cm.s-1*	*Viscosity η.10^3 poise*
	DMF			DMSO		
ANC-1						
0.00	0.9337	1.4308	7.2751	1.0846	1.4604	16.5573
0.01	0.9372	1.4316	7.3778	1.0847	1.4608	16.9630
0.02	0.9383	1.4328	7.4699	1.0848	1.4612	17.0657
0.04	0.9399	1.4328	7.5423	1.085	1.4628	17.2434
0.06	0.9408	1.4360	7.6611	1.0854	1.4628	17.3003
0.08	0.9423	1.4368	7.7571	1.0858	1.4632	17.3527

0.10	0.9438	1.4408	7.8894	1.0868	1.4664	17.5251
ANC-2						
0.01	0.9363	1.4320	7.3152	1.0848	1.4680	17.8006
0.02	0.9370	1.4348	7.3603	1.0849	1.4688	17.9631
0.04	0.9372	1.4360	7.4373	1.0856	1.4732	18.1724
0.06	0.9374	1.4388	7.4826	1.0865	1.4748	18.2886
0.08	0.9384	1.4440	7.5700	1.0875	1.4752	18.3884
0.10	0.9405	1.4488	7.6547	1.0887	1.4768	18.7221
ANC-3						
0.01	0.9376	1.4320	7.3214	1.0849	1.4676	17.8758
0.02	0.9391	1.4320	7.4206	1.0853	1.4720	18.1719
0.04	0.9401	1.4336	7.4564	1.0866	1.4756	18.4376
0.06	0.9407	1.4360	7.5647	1.0881	1.4828	19.0482
0.08	0.9427	1.4380	7.6885	1.0922	1.4892	19.8600
0.10	0.9491	1.4388	7.8292	1.0952	1.4936	20.1557
ANC-4						
0.01	0.9376	1.4316	7.3373	1.0849	1.4648	17.0534
0.02	0.9394	1.4324	7.4230	1.0863	1.4660	17.2641
0.04	0.942	1.4344	7.4914	1.0876	1.4664	17.3492
0.06	0.9451	1.4372	7.5961	1.0888	1.4696	17.5804
0.08	0.9464	1.4428	7.7027	1.0906	1.4700	18.1683
0.10	0.9493	1.4444	7.7786	1.0921	1.4700	18.4245
ANC-5						
0.01	0.9374	1.4324	7.7088	1.0847	1.4636	16.8115
0.02	0.9398	1.4336	7.7723	1.0848	1.4640	16.9738
0.04	0.9401	1.4368	7.8226	1.0859	1.4648	17.0600
0.06	0.9403	1.4396	7.8561	1.0865	1.4652	17.1844
0.08	0.9409	1.4444	7.9289	1.0872	1.4668	17.2830
0.10	0.9442	1.4468	8.0686	1.0880	1.4696	17.4708
ANC-6						
0.01	0.9399	1.4332	7.6657	1.0847	1.4652	17.9873
0.02	0.9423	1.4368	8.0284	1.0847	1.4656	18.1711
0.04	0.9438	1.4420	8.2730	1.0848	1.4664	18.3289
0.06	0.9469	1.4472	8.7974	1.0848	1.4672	18.4484
0.08	0.9485	1.4504	9.2862	1.0860	1.4684	18.6527
0.10	0.9514	1.4532	9.4153	1.0915	1.4696	18.8951
ANC-7						
0.01	0.9385	1.4312	7.5152	1.0858	1.4652	17.8952
0.02	0.9392	1.4328	7.6282	1.0867	1.4656	17.2782
0.04	0.9405	1.4344	7.7941	1.0876	1.4676	18.4914
0.06	0.9418	1.4380	7.9325	1.0880	1.4720	18.8069
0.08	0.9440	1.4392	8.1349	1.0888	1.4724	18.9313
0.10	0.9467	1.4436	8.4147	1.0895	1.4736	19.0819
ANC-8						
0.01	0.9375	1.4324	7.5151	1.0847	1.4636	16.9630
0.02	0.9388	1.4376	7.6369	1.0854	1.4636	17.0935
0.04	0.9397	1.4408	7.6999	1.0859	1.4640	17.2255
0.06	0.9410	1.4464	7.8978	1.0870	1.4644	17.4547
0.08	0.9434	1.4484	8.0099	1.0879	1.4652	17.6120
0.10	0.9457	1.4548	8.0975	1.0887	1.4664	17.8600
ANC-9						

0.01	0.9372	1.4316	7.3341	1.0858	1.4640	17.2055
0.02	0.9390	1.4320	7.4198	1.0867	1.4652	17.8180
0.04	0.9414	1.4332	7.4746	1.0871	1.4672	18.0179
0.06	0.9448	1.4336	7.5776	1.0882	1.4676	18.8564
0.08	0.9465	1.4368	7.7075	1.0889	1.4684	19.1683
0.10	0.9484	1.4384	7.8073	1.0900	1.4692	19.4184

Table 3. Some acoustical parameters of Chalocones in DMF at 308.15K.

Conc. M	$Z.10^{-5}$ $g.cm^{-2}$	π	$R_m.10^{-3}$ $cm^{-8/3}.s^{-1/3}$	b $cm^3.mol^{-1}$	r
0.00	1.3359	483.16	4.0943	78.2781	0.2003
0.01	1.3417	481.06	4.1275	78.8983	0.1994
0.02	1.3444	477.80	4.1714	79.7150	0.1981
0.04	1.3467	468.20	4.2591	81.3908	0.1981
0.06	1.3510	459.70	4.3528	83.1205	0.1945
0.08	1.3539	451.50	4.4408	84.7848	0.1936
0.10	1.3598	444.23	4.5316	86.4382	0.1891
ANC-2					
0.01	1.3408	478.55	4.1326	78.9880	0.1990
0.02	1.3444	473.31	4.1806	79.8543	0.1958
0.04	1.3458	463.10	4.2778	81.6879	0.1945
0.06	1.3487	452.15	4.3766	83.5200	0.1913
0.08	1.3550	442.87	4.4737	85.2714	0.1855
0.10	1.3626	434.40	4.5644	86.9027	0.1801
ANC-3					
0.01	1.3426	475.98	4.1507	79.3344	0.1990
0.02	1.3448	470.16	4.2160	80.5830	0.1990
0.04	1.3477	453.27	4.3568	83.2434	0.1972
0.06	1.3508	439.42	4.5001	85.9324	0.1945
0.08	1.3556	427.49	4.6349	88.4667	0.1922
0.10	1.3656	418.59	4.7420	90.4941	0.1913
ANC-4					
0.01	1.3423	479.69	4.1271	78.8904	0.1994
0.02	1.3456	476.38	4.1687	79.6717	0.1985
0.04	1.3512	466.40	4.2562	81.3049	0.1963
0.06	1.3583	458.10	4.3410	82.8722	0.1931
0.08	1.3655	449.20	4.4368	84.5918	0.1868
0.10	1.3712	441.04	4.5197	86.1407	0.1850
ANC-5					
0.01	1.3427	490.70	4.1344	79.0157	0.1985
0.02	1.3473	485.86	4.1793	79.8525	0.1972
0.04	1.3507	472.60	4.2901	81.9076	0.1936
0.06	1.3537	459.57	4.4009	83.9696	0.1904
0.08	1.3590	448.17	4.5118	85.9897	0.1850

0.10	1.3661	440.56	4.6053	87.7234	0.1823
ANC-6					
0.01	1.3471	483.16	4.1281	78.8802	0.1976
0.02	1.3539	489.51	4.1791	79.7892	0.1936
0.04	1.3610	493.06	4.2937	81.8774	0.1877
0.06	1.3704	484.39	4.3997	83.7989	0.1819
0.08	1.3757	484.50	4.5103	85.8429	0.1783
0.10	1.3826	472.97	4.6129	87.7378	0.1751
ANC-7					
0.01	1.3432	486.00	4.1217	78.7942	0.1999
0.02	1.3457	483.06	4.1680	79.6499	0.1981
0.04	1.3491	475.72	4.2592	81.3624	0.1963
0.06	1.3543	467.56	4.3519	83.0651	0.1922
0.08	1.3586	462.30	4.4373	84.6705	0.1909
0.10	1.3667	459.04	4.5225	86.2097	0.1859
ANC-8					
0.01	1.3429	484.72	4.1325	78.9796	0.1985
0.02	1.3496	480.98	4.1849	79.8847	0.1927
0.04	1.3539	468.81	4.2902	81.8342	0.1891
0.06	1.3611	461.02	4.3957	83.7380	0.1828
0.08	1.3664	452.11	4.4914	85.5216	0.1805
0.10	1.3758	442.29	4.5914	87.2964	0.1733
ANC-9					
0.01	1.3417	476.92	4.1476	79.2824	0.1994
0.02	1.3446	471.28	4.2075	80.4197	0.1990
0.04	1.3492	456.56	4.3321	82.7784	0.1976
0.06	1.3545	444.76	4.4495	85.0138	0.1972
0.08	1.3599	433.48	4.5772	87.3901	0.1936
0.10	1.3642	422.39	4.7014	89.7271	0.1918

Table 4. Some acoustical parameters of Chalcones in DMSO at 303.15 K.

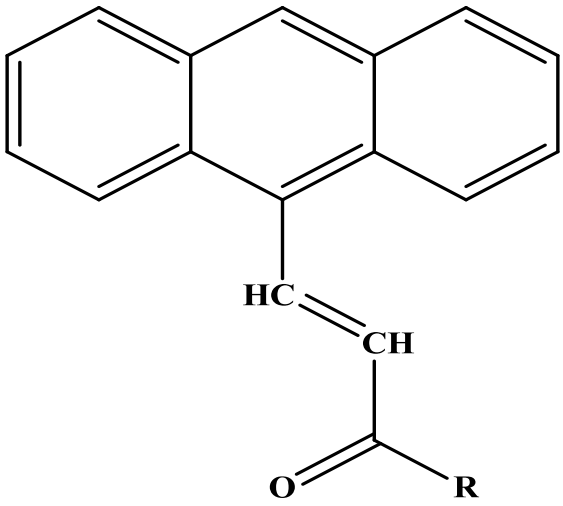
Conc. M	$Z.10^{-5}$ $g.cm^{-2}$	π	$R_m.10^{-3}$ $cm^{-8/3}.s^{-1/3}$	b $cm^3.mol^{-1}$	r
ANC-1					
0.00	1.5839	737.58	3.7935	72.0341	0.1669
0.01	1.5845	738.52	3.8286	72.6949	0.1664
0.02	1.5851	732.84	3.8638	73.3554	0.1660
0.04	1.5871	721.00	3.9348	74.6757	0.1641
0.06	1.5877	707.62	4.0035	75.9803	0.1641
0.08	1.5887	694.55	4.0725	77.2830	0.1637
0.10	1.5937	683.95	4.1416	78.5366	0.1600
ANC-2					
0.01	1.5925	754.60	3.8351	72.6978	0.1582
0.02	1.5935	749.73	3.8711	73.3679	0.1573
0.04	1.5993	737.40	3.9438	74.6715	0.1522

0.06	1.6024	724.48	4.0132	75.9571	0.1504
0.08	1.6043	712.07	4.0808	77.2307	0.1499
0.10	1.6078	704.37	4.1486	78.4838	0.1481
ANC-3					
0.01	1.5922	752.25	3.8522	73.0298	0.1587
0.02	1.5976	745.41	3.9082	74.0173	0.1536
0.04	1.6034	727.26	4.0136	75.9511	0.1495
0.06	1.6134	715.86	4.1211	77.8600	0.1411
0.08	1.6265	710.01	4.2166	79.5491	0.1337
0.10	1.6358	695.34	4.3138	81.3024	0.1286
ANC-4					
0.01	1.5892	739.33	3.8324	72.7008	0.1619
0.02	1.5925	736.12	3.8646	73.2909	0.1605
0.04	1.5949	722.68	3.9323	74.5679	0.1600
0.06	1.6001	712.03	4.0026	75.8460	0.1564
0.08	1.6032	709.73	4.0677	77.0728	0.1559
0.10	1.6054	701.03	4.1332	78.3145	0.1559
ANC-5					
0.01	1.5876	733.33	3.8363	72.7945	0.1632
0.02	1.5881	727.86	3.8767	73.5546	0.1628
0.04	1.5906	712.66	3.9541	75.0091	0.1619
0.06	1.5919	698.79	4.0328	76.4949	0.1614
0.08	1.5947	684.76	4.1121	77.9696	0.1596
0.10	1.5989	672.81	4.1919	79.4325	0.1564
ANC-6					
0.01	1.5893	757.43	3.8408	72.8522	0.1614
0.02	1.5897	751.26	3.8846	73.6768	0.1609
0.04	1.5908	735.12	4.9719	75.3189	0.1600
0.06	1.5916	718.91	4.0596	76.9680	0.1591
0.08	1.5947	705.54	4.1427	78.5228	0.1577
0.10	1.6041	*695.60*	4.2072	79.7230	0.1564
ANC-7					
0.01	1.5909	757.85	3.8288	72.6254	0.1614
0.02	1.5927	758.08	3.8613	73.2344	0.1609
0.04	1.5962	746.46	3.9303	74.5100	0.1587
0.06	1.6015	736.44	4.0033	75.8180	0.1536
0.08	1.6031	724.26	4.0710	77.0937	0.1531
0.10	1.6055	712.78	4.1397	78.3733	0.1518
ANC-8					
0.01	1.5876	736.87	3.8353	72.7740	0.1632
0.02	1.5886	731.27	3.8720	73.4722	0.1632
0.04	1.5898	717.22	3.9491	74.9274	0.1628
0.06	1.5918	706.01	4.0237	76.3354	0.1623
0.08	1.5940	693.65	4.0991	77.7528	0.1614
0.10	1.5965	683.38	4.1752	79.1734	0.1600
ANC-9					
0.01	1.5896	740.09	3.8425	72.9045	0.1628

0.02	1.5922	741.99	3.8903	73.7917	0.1614
0.04	1.5950	724.07	3.9906	75.6593	0.1591
0.06	1.5970	720.10	4.0865	77.4706	0.1587
0.08	1.5989	706.04	4.1841	79.3062	0.1577
0.10	1.6014	691.75	4.2797	81.1039	0.1568

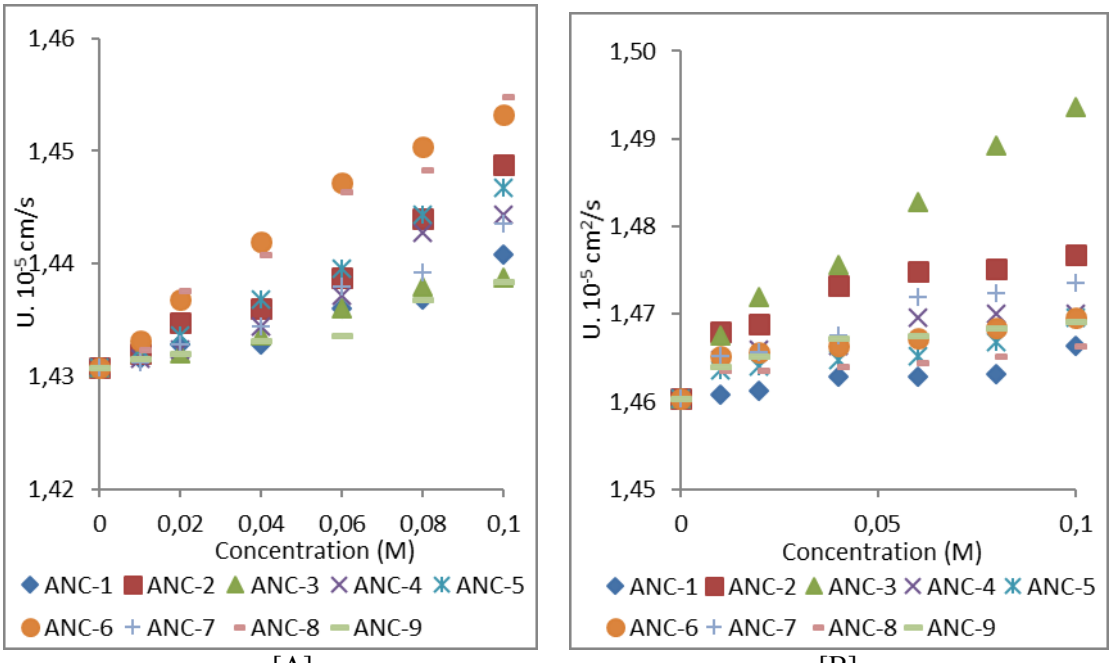
Table 5. The Bachem's constants A and B, ϕ^{o}_{k} and S_k, Φ_V^{o} and S_v of Chalcones in DMF and DMSO at 303.15 K.

Comp.	$A\ X\ 10^{11}$ $dyn^{-1}.cm^{3}$ mol^{-1}	$B\ X\ 10^{11}$ $dyn^{-1}.cm^{-1/2}$ $mol^{-3/2}$	$\phi^{o}_{k}\ X\ 10^{8}$ $dyn^{-1}.mol^{-1}$	$S_k\ X\ 10^{8}$ $dyn^{-1}cm^{-3/2}$ $mol^{-3/2}$	Φ_V^{o} $cm^{2}.\ mol^{-1}$	S_v $cm^{2}.dm^{1/2}$ $.mol^{-3/2}$
DMF						
ANC-1	-1.70	2.04	-0.80	2.70	-124.0	1040.00
ANC -2	-2.56	3.53	-3.00	10.60	-44.0	1777.78
ANC -3	-2.40	4.60	-1.30	5.93	-290.0	4206.89
ANC -4	-2.40	3.24	-1.75	3.00	-176.0	975.00
ANC -5	-4.25	10.71	-5.00	1.65	-386.0	7142.85
ANC -6	-4.60	6.33	-5.40	12.50	-262.0	1900.00
ANC -7	-3.60	9.09	-1.74	4.89	-74.0	225.35
ANC -8	-3.56	4.76	-2.32	1.56	-57.0	178.08
ANC -9	-2.20	3.44	-1.20	3.47	-164.0	1027.00
DMSO						
ANC -1	-0.26	0.10	-0.35	10.36	71.00	127.27
ANC -2	-3.65	8.75	-2.35	7.82	53.00	150.00
ANC -3	-4.60	7.45	-2.85	11.40	55.00	716.66
ANC -4	-2.88	6.53	-1.26	5.25	-13.00	410.71
ANC -5	-1.60	3.73	-0.03	0.38	43.00	61.53
ANC -6	-2.75	8.64	-1.14	7.68	65.50	266.66
ANC -7	-2.90	7.29	-1.22	4.10	-46.60	928.57
ANC -8	-1.00	1.76	-0.34	1.18	35.00	425.00
ANC -9	-2.06	4.32	-1.08	2.62	9.00	220.93



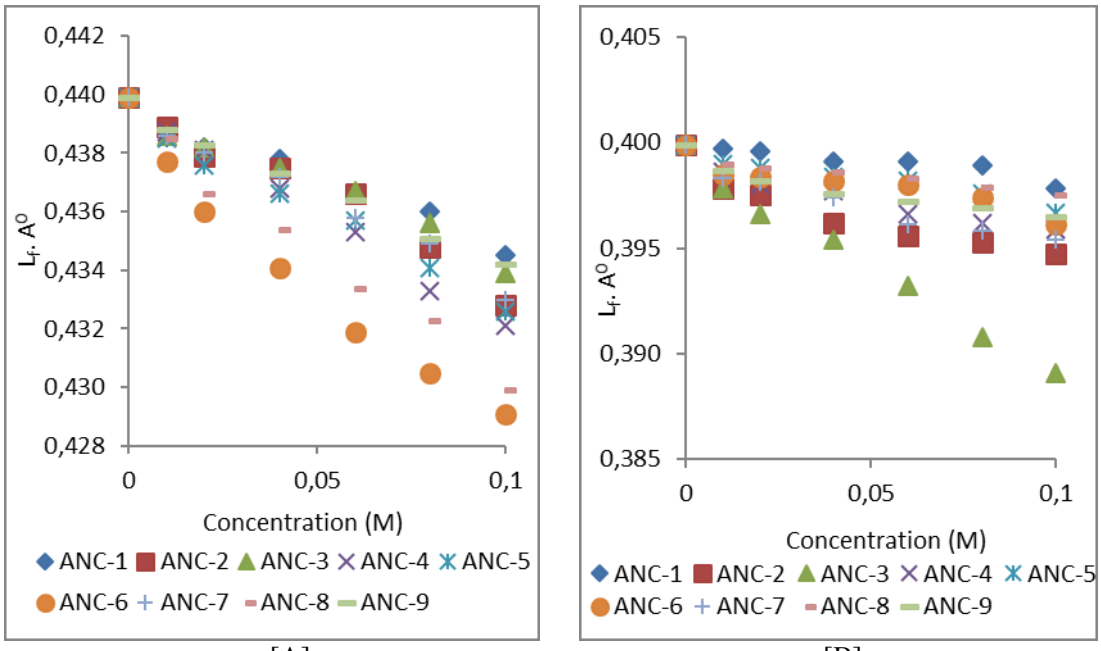
R = Aryl

Fig. 1. General structure of Chalcone.



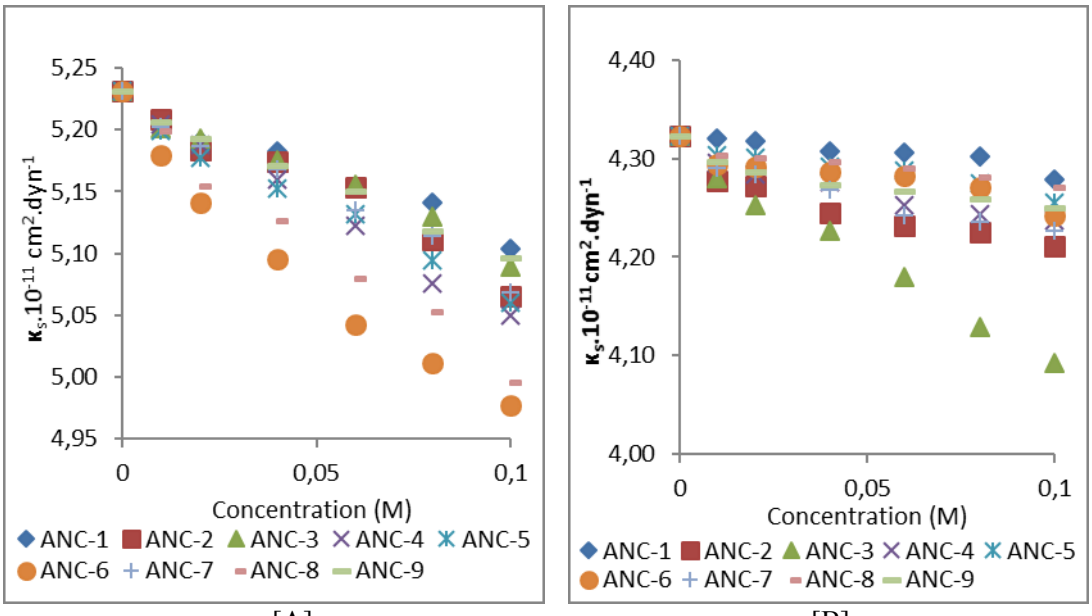
[A] [B]

Fig. 2. Variation of ultrasonic velocity with concentration of Chalcones in [A] DMF and [B] DMSO at 303.15 K.



[A] [B]

Fig. 3. Variation of intermolecular free path length (L_f) with concentration of Chalcones in [A] DMF and [B] DMSO at 303.15 K.



[A] [B]

Fig. 4. Variation of adiabatic compressibility (κ_s) with concentration of of Chalcones in [A] DMF and [B] DMSO at 303.15 K.

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(Received 02 December 2014; accepted 13 December 2014)